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Electronic Supplementary Information

Tuning Twist Angle of Thermally Activated Delayed Fluorescence Molecules via Dendronization Strategy: High-Efficiency Solution-Processed Non-Doped OLEDs

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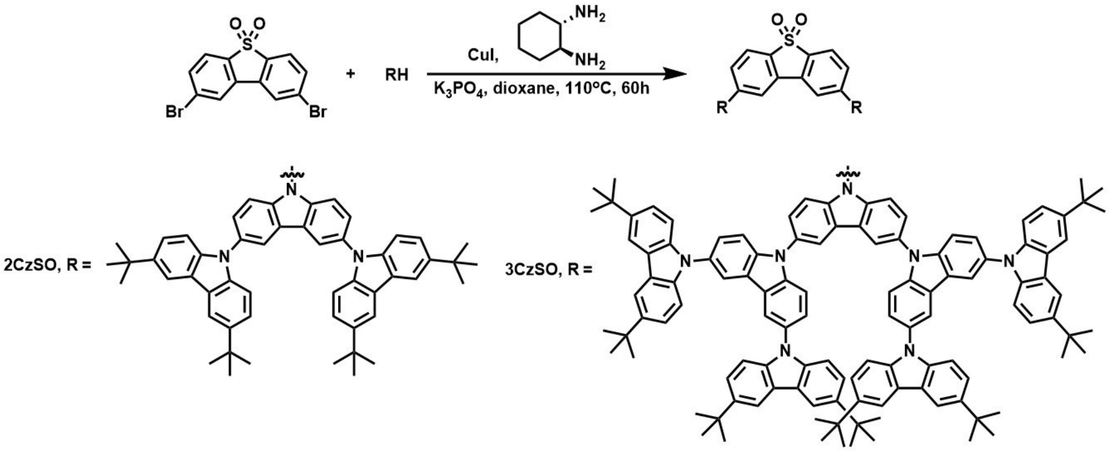
Experimental Section

General information: All chemicals reagents from commercial sources were directly used without further purification. Solvents used to synthesize were purified according to standard procedures before used. ^{1}H NMR and ^{13}C NMR spectra were recorded with a MERCURYVX300 or Bruker Advanced II (400 MHz) spectrometers. Matrix-assisted laser desorption ionization/time-of-flight (MALDI-TOF) mass spectra were performed on a Bruker BIFLEX III TOF mass spectrometer. Elemental analysis of carbon, hydrogen, and nitrogen were measured by a Vario EL Ш microanalyzer. UV-vis absorption spectra and photoluminescence (PL) spectra were recorded by a Shimadzu UV-2700 recording spectrophotometer and a Hitachi F-4600 fluorescence spectrophotometer. The Phosphorescence spectra were measured by a Hitachi F-4600 fluorescence spectrophotometer with a low temperature accessory. Absolute PLQYs were obtained using a Quantaurus-QY measurement system (C11347-11, Hamamatsu

Photonics) and all the samples were excited at 310 nm. The PLQYs under oxygen-free were calculated through relative method measured by Hitachi F-4600 fluorescence spectrophotometer. Thermogravimetric analysis (TGA) was measured by a NEZSCH STA 449C instrument at a rate of 15 ^{o}C min^{-1} from 25 ^{o}C to 800 ^{o}C under nitrogen atmosphere. Differential scanning calorimetry (DSC) was performed with a NETZSCH DSC 200 PC unit at a heating rate of 10 ^{o}C min^{-1} from room temperature to 300 ^{o}C under argon. Cyclic voltammetry (CV) was operated in nitrogen-purged dichloromethane (oxidation scan) at room temperature with CHI voltammetric analyzer. Tetrabutylammonium hexaflorophosphate ($TBAPF_6$) (0.1M) was regarded as the supporting electrolyte. The conventional three-electrode configuration consists of a platinum working electrode, a platinum wire auxiliary electrode, and an Ag wire pseudoreference electrode with ferrocenium-ferrocene (Fc^+/Fc) as the internal standard. Cyclic voltammograms were obtained at a scan rate of 100 mV s^{-1}. The onset potential was determined from the intersection of two tangents drawn at the rising and background current of the cyclic voltammogram.

Device fabrication and characterizations: The indium tin oxide (ITO) was coated on glass substrates with a sheet resistance of 15-20 ohm/square, cleaned in an ultrasonic bath, and then treated with UV-Ozone for 20 min. A 30 nm thick layer of PEDOT:PSS (Baytron P 4083, Bayer AG) used as a hole-injecting layer was spin-coated on the ITO substrate and then baked inside the glove-box at 120 ^{o}C for 10 min. The EML was prepared by spin-coating from chlorobenzene solution on top of the PEDOT:PSS layer and annealed at 80 ^{o}C. The Electron-transporting material was thermally evaporated onto the emitter layer in a vacuum chamber at a pressure less than 3.0×10^{-4} Pa. And then a 1 nm thick layer of Liq as electron injection layer was evaporated. Finally, Al was subsequently deposited through a shadow mask successively to define the size of the active area. Except for the spin-coating of the PEDOT:PSS layer, all the processes were carried out in the controlled atmosphere of a nitrogen dry-box (Vacuum Atmosphere Co.) containing less than 0.1 ppm oxygen and moisture. The devices were encapsulated with UV-curable epoxy before taken out from the glove-box. All the measurements were carried out at room temperature under ambient conditions.



Scheme S1. Synthetic routes of the two dendrimers.

Table S1. Thermal, photophysical, theoretical calculation data of the materials

Compound	T_d [°C]	λ_{abs} [nm]$^{a)}$	FWHM [nm]	k_p [10^7 s^{-1}]$^{b)}$	k_{ISC} [10^6 s^{-1}]$^{c)}$
2CzSO	510	289,298,336,349	84	1.24	3.10
3CzSO	500	289,298,336,349	95	0.25	0.79

[a)] Measured in the film; [b)] The rate constant of prompt fluorescence process; [c)] The rate constant of ISC process.

Table S2. EL performances of the devices

Device	CIE(x, y)$^{a)}$
A1	(0.18, 0.19)
A2	(0.24, 0.49)
A3	(0.29, 0.52)
B1	(0.27, 0.52)
B2	(0.24, 0.49)
C1	(0.31,0.53)

[a)] the Commission Internationale de L'Eclairage (CIE) coordinates.

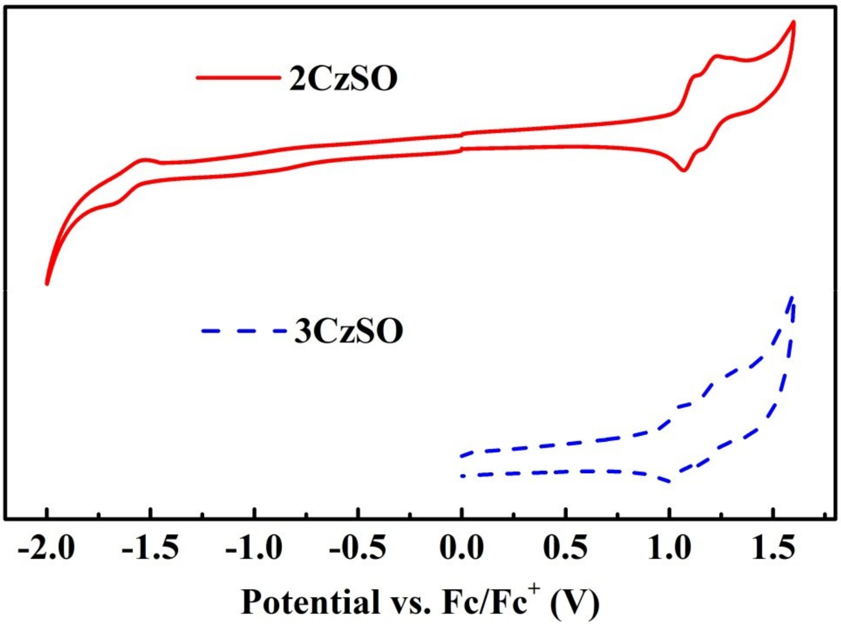


Fig. S1. Cyclic voltammograms of the materials in CH_2Cl_2.

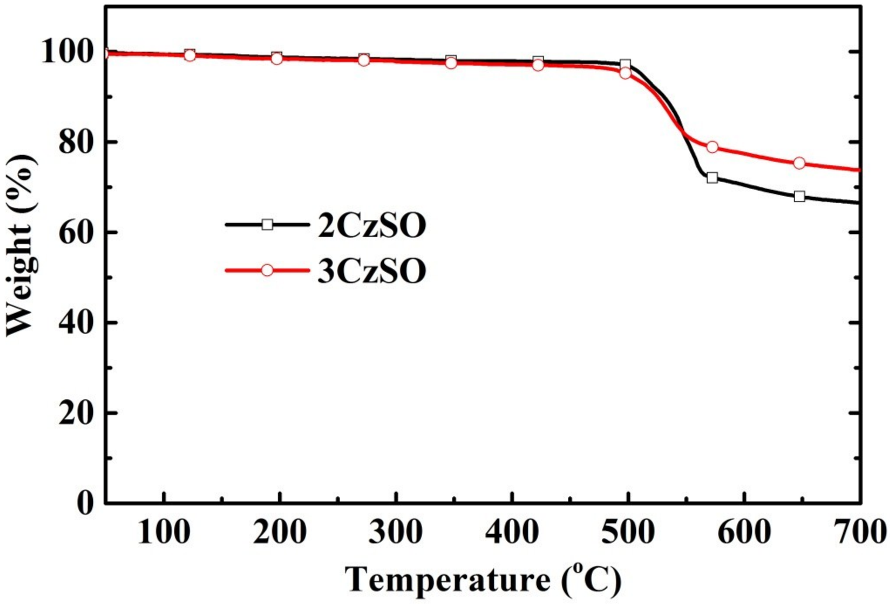


Fig. S2. TGA traces of **2CzSO** and **3CzSO**.

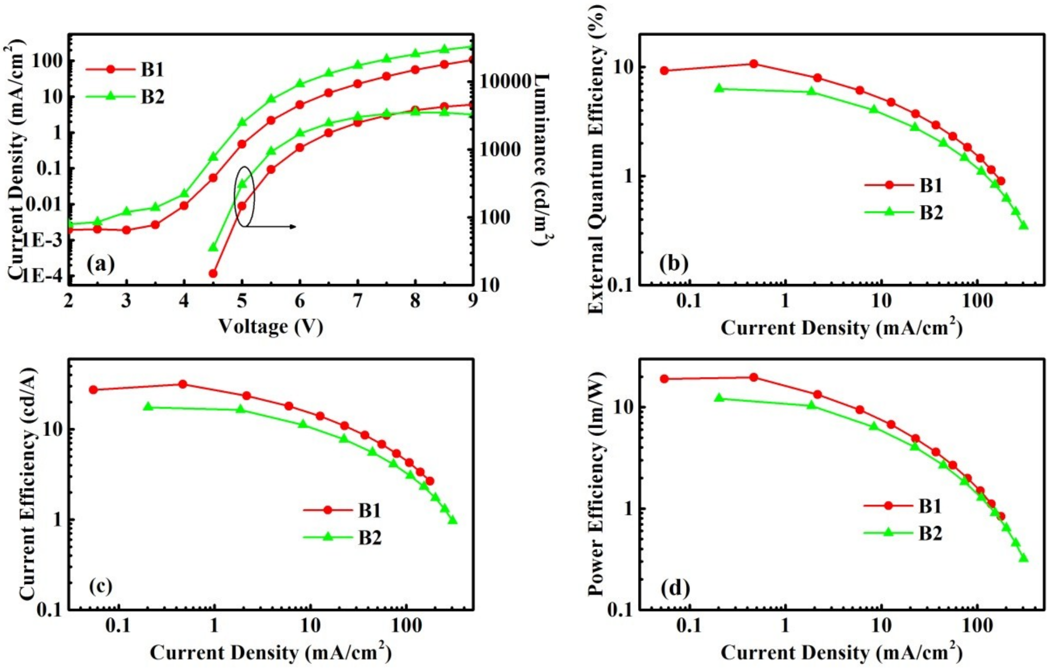


Fig. S3. (a) Current density−voltage−luminance (*J*−*V*−*L*) characteristics, (b) power efficiency versus luminance curves, (c) current efficiency versus luminance curves and (d) external quantum efficiency versus luminance curves for devices B1 and B2.

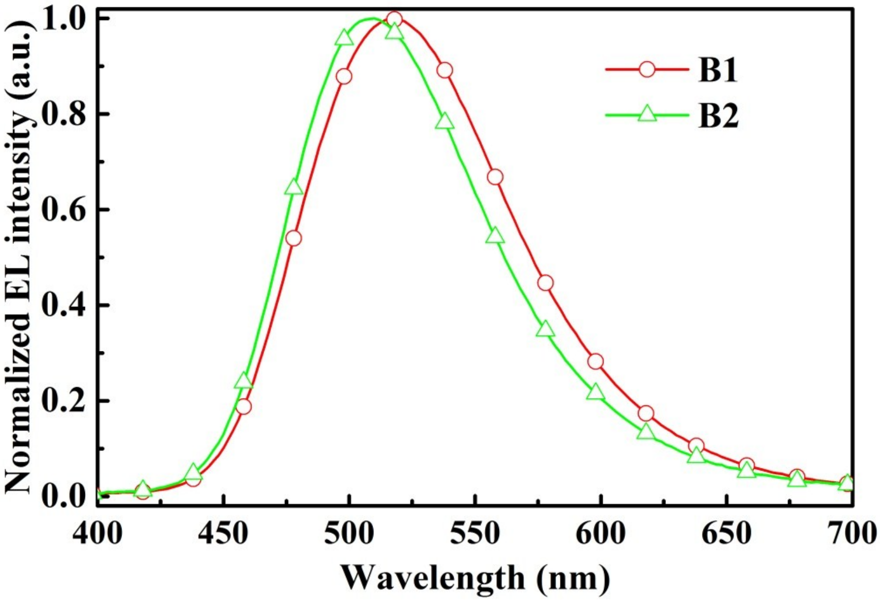


Fig. S4. Normalized EL spectra of devices B1-B2.

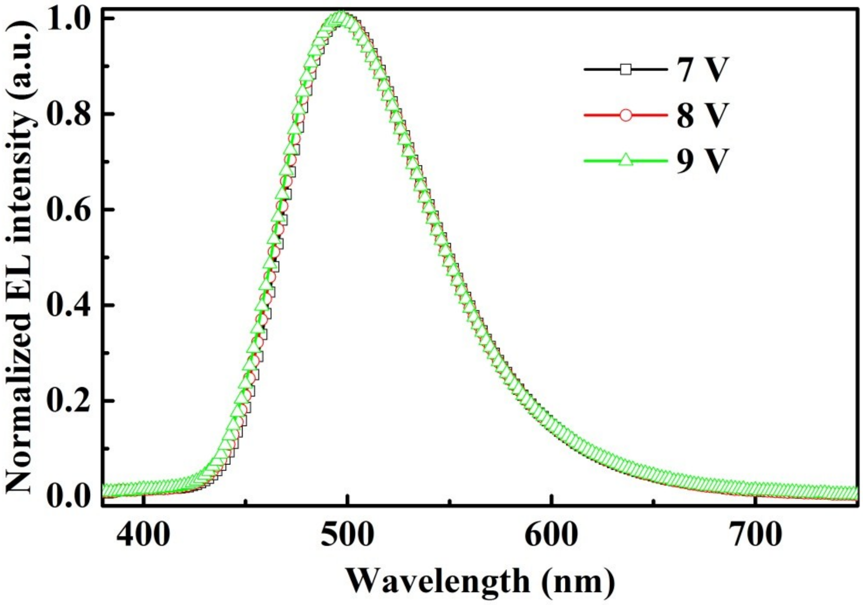


Fig. S5. Normalized EL spectra of the single layer device of ITO/PEDOT:PSS/**2CzSO**/Liq/Al under different operating voltages.

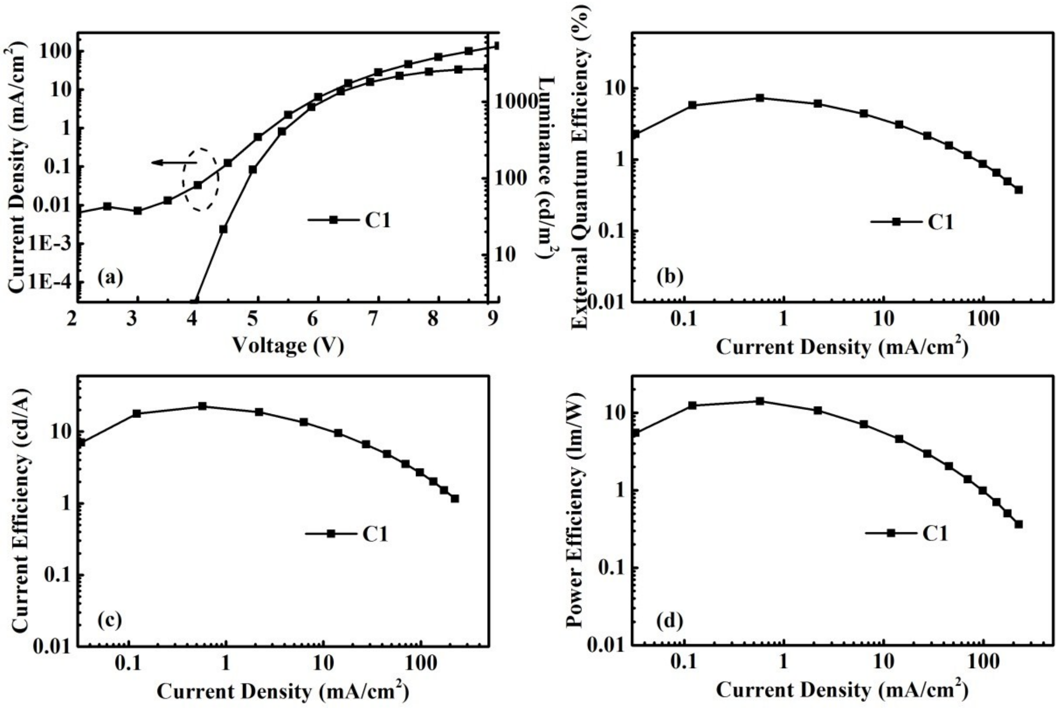


Fig. S6. (a) Current density−voltage−luminance (J−V−L) characteristics, (b) power efficiency versus luminance curve, (c) current efficiency versus luminance curve, and (d) external quantum efficiency versus luminance curve for device C1.

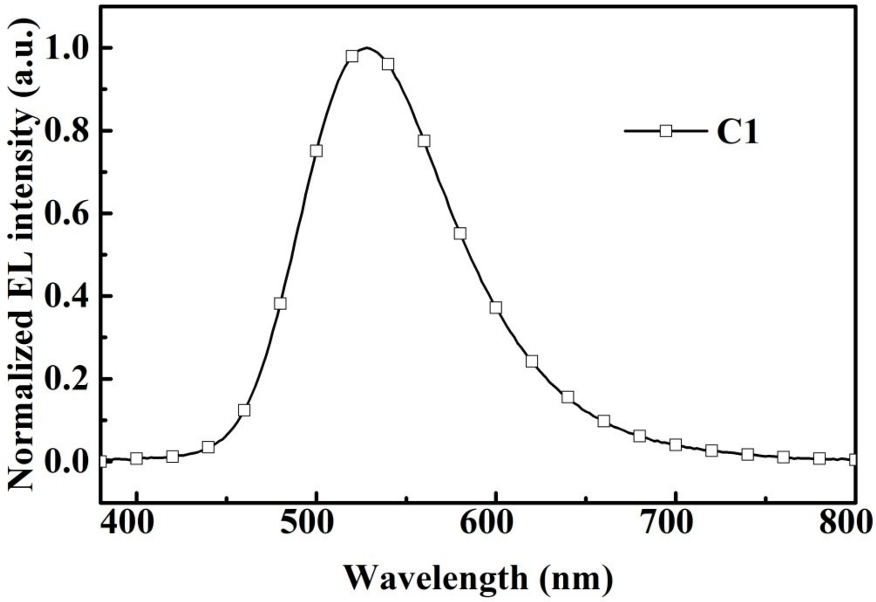


Fig. S7. Normalized EL spectrum of device C1.

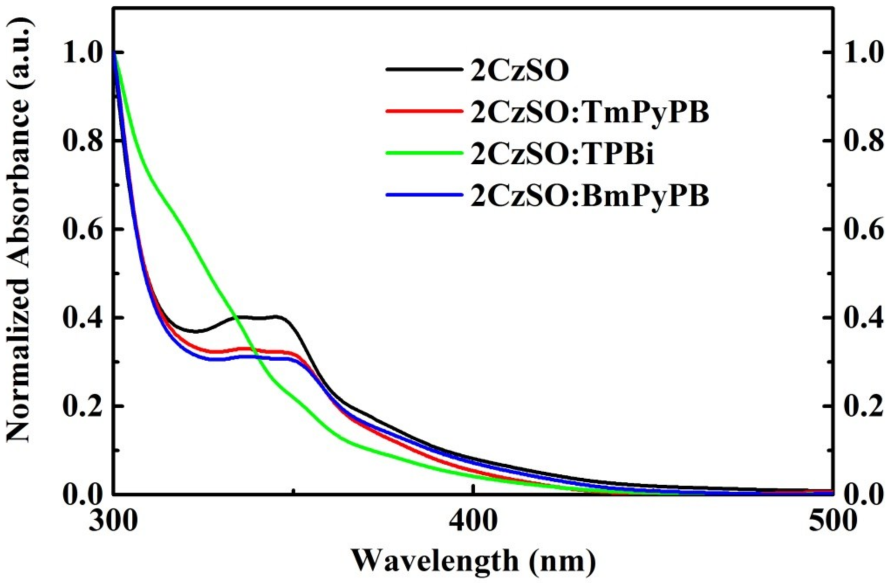


Fig. S8. The absorption spectra of the neat film of 2CzSO, the mixed films of 2CzSO:TmPyPB, 2CzSO:TPBi, and 2CzSO:BmPyPB at room temperature.

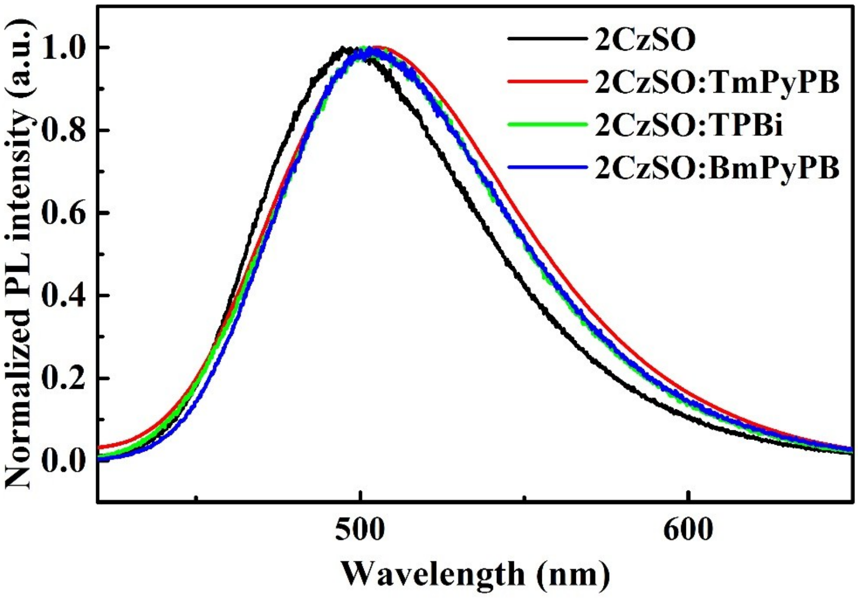


Fig. S9. The fluorescence spectra of the neat film of 2CzSO, the mixed films of 2CzSO:TmPyPB, 2CzSO:TPBi, and 2CzSO:BmPyPB at room temperature.

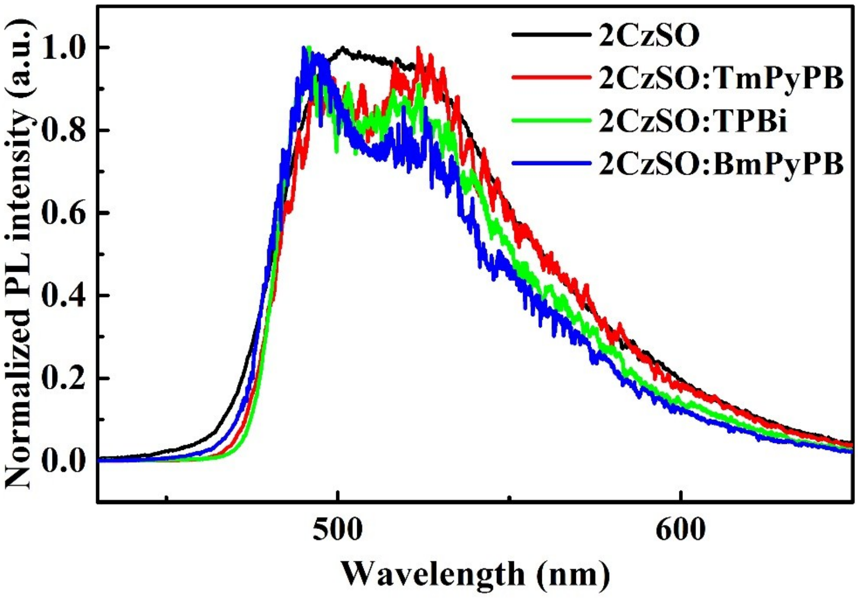


Fig. S10. The phosphorescence spectra of the neat film of 2CzSO, the mixed films of 2CzSO:TmPyPB, 2CzSO:TPBi, and 2CzSO:BmPyPB at 77 K.

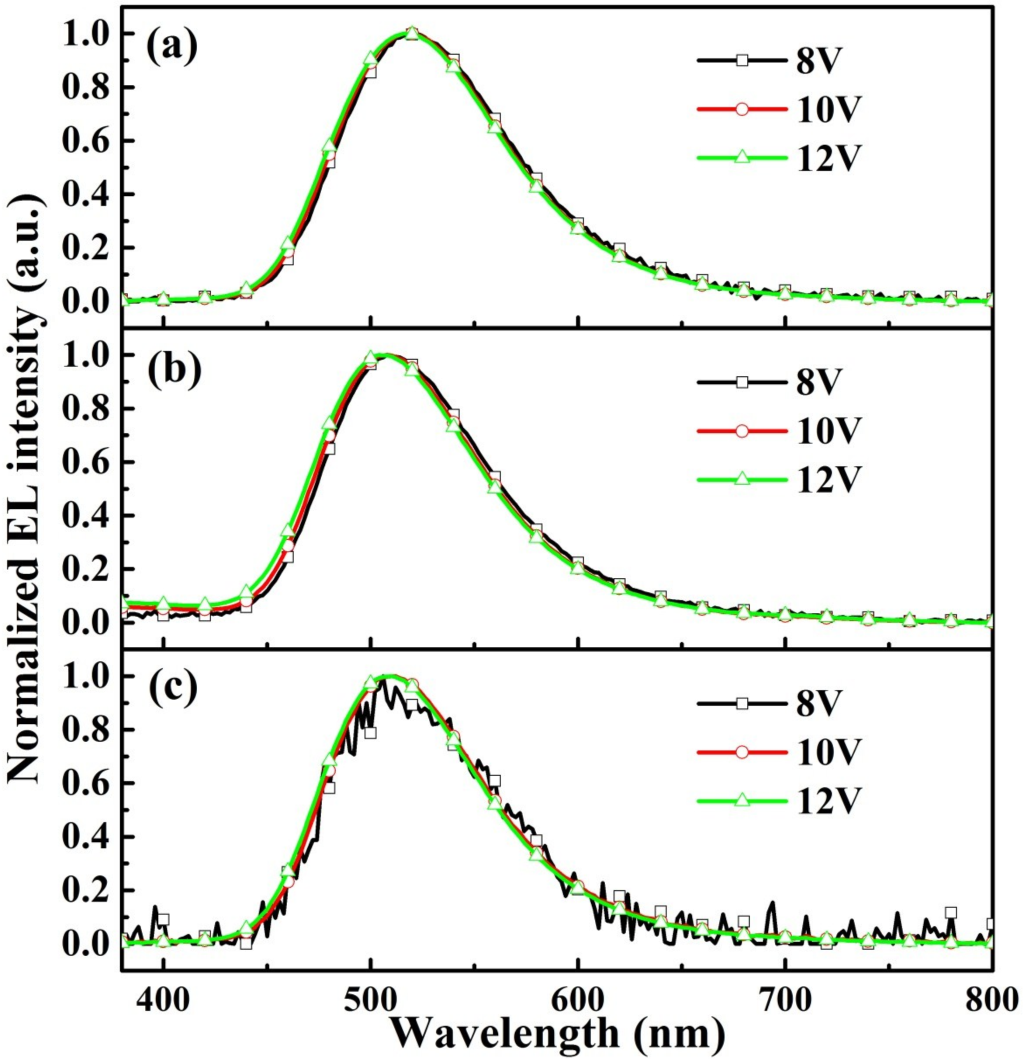


Fig. S11. The EL spectra of the devices A2 (a), B1 (b) and B2 (c) at 8, 10 and 12 V, respectively.

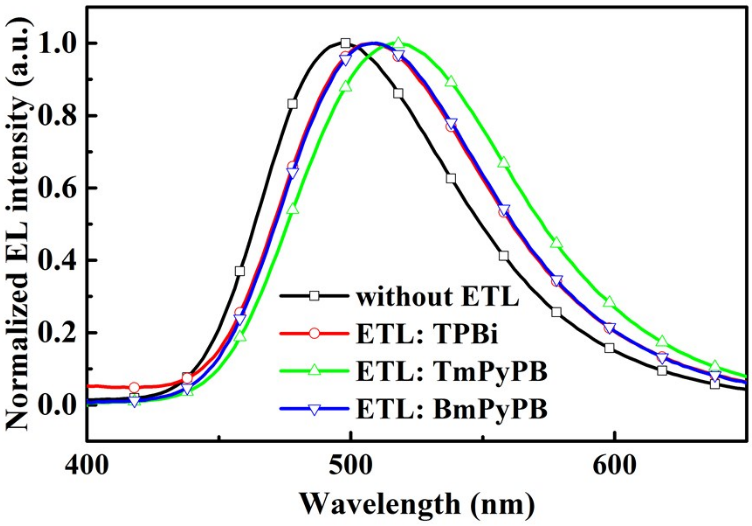


Fig S12. The EL spectra of the devices without and with the ETLs of TPBi, TmPyPB and BmPyPB.